BLACKBOX MODELLING OF FUEL CELL COMPONENTS WITHOUT MATHEMATICAL SOLVERS FOR REAL TIME SIMULATION WITH REDUCED ORDER MODEL APPROACH FOR WEB APPLICATION

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ABSTRACT: Simulation software is one of the key factors in developing and optimizing new and existing energy system and components. Due to the system requirements and the cost of these software a new open-source software is presented in this article. It is depending on the Mean-Value-Modelling approach, which is used for black box modelling of different key components of fuel cell systems. In combination with a web-based interface this software is able to perform simulations in real time.

KEYWORDS: simulation, open-source, python, black box modelling, fuel cell system.

1 INTRODUCTION

Simulation is a major part of developing and optimizing existing technologies as well as develop new technologies. For this reason, different simulation software are already distributed in the market. The biggest flaws of these simulation software are the high cost as well as the interoperability between each software and the high numerical demands. Therefore, in this paper a new approach of black box modelling is introduced to overcome these major flaws of existing software and present a new simulation software based on python.

The methodology applied for developing black box models of fuel cell components is based on the modelling approach of [1] and [2]. The approach of both is based on “control oriented model” (COM) approach. This approach represents all dynamic (transient) process of the modelled component [2]. For this work the “Mean-Value” modelling (MVM) of COM components is used. MVM is a continuous model approach, which neglect discrete cycles and assume that all processes and effects take place over calculation cycles [2, S. 23]. The used MVMs in this work are therefore divided into two classes mainly called reservoirs and flows. This differentiation is caused by the use of the “lumped parameter system” (LPS) and describes the behaviour of the flow between the reservoirs and the behaviour of the fluid in each reservoir with ordinary differential equations. The LPS divides the system to be simulated in reservoirs according to the simulation time. To be able to simulate the model without mathematical solver the modelling approaches are integrated into the object-oriented program language python. Therefore, different classes in python are build due to the following modelling approaches.

For the proof of concept of this simulation the cathode system of a fuel system is simulated, by integrating the fuel cell cathode, the cathode compressor and two pressure valves. Therefore, the methodical approach on the basics of the simulation, flow and reservoir components, as well as the cathode side of the fuel cell and the compressor model approach are analysed (Figure 1). Focus of this work is to present overview of the concept and usability of this approach on web-based applications. The usability of the simulation is checked by plausibility according to the runtime of the mentioned system and the time dependent behaviour of the system.

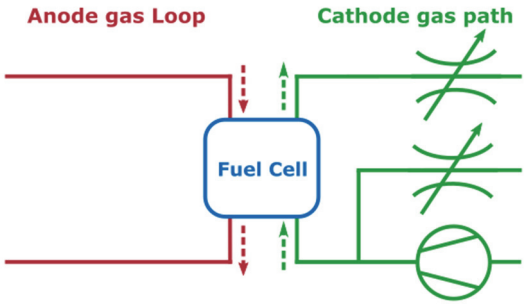

Figure 1: System for validation of simulation approach.

2 MODELLING OF RESERVOIRS

Modelling the reservoir of system, the inputs and outputs of mass flow, enthalpy flow and the temperature of reservoir before and after the current reservoir are necessary for calculating the change in pressure and temperature.

The mentioned inputs and outputs are shown in Figure 2. In the black box of the reservoir the following states are calculated by the following differential equations. In equation 1 the change in pressure $\frac{dP}{dt}$ is calculated by

$$\frac{dp}{dt} = \frac{\kappa \cdot R}{V} \cdot (\dot{m}_{in} \cdot T_{in} - \dot{m}_{out} \cdot T). \quad (1)$$

Equation 2 calculates the change in temperature $\frac{dT}{dt}$ as follows:

$$\frac{dT}{dt} = \frac{T \cdot R}{p \cdot V \cdot c_v} \cdot (c_p \cdot \dot{m}_{in} \cdot T_{in} - c_p \cdot \dot{m}_{out} \cdot T - c_v \cdot (\dot{m}_{in} - \dot{m}_{out}) \cdot T) \quad (2)$$

Both equations describe the relationship between the volume of the reservoir, the mentioned inputs and the medium flowing through the reservoir [2].

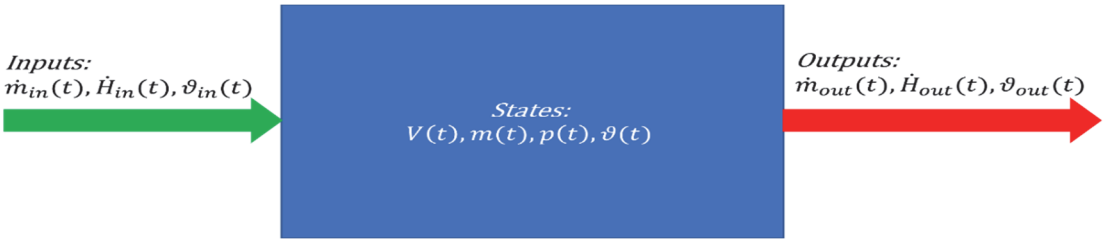

Figure 2: Inputs, outputs and states of reservoir.

3 MODELLING OF FLOWS

Due to the insignificant pressure loss between two reservoirs, the medium is assumed to be incompressible [1]. Under this assumption the following equation is used to calculate the mass flow between two reservoirs:

$$\dot{m}_{in,out} = \lambda_{laminar} \cdot A_{crosssection} \cdot \sqrt{\frac{2 \cdot p_1}{R \cdot T}} \cdot \sqrt{(p_2 - p_1)} \tag{3}$$

Due to the possibility of back flows equation 3 is extended in equation 4.

$$\dot{m}_{in,out} = \frac{p_2 - p_1}{|(p_2 - p_1)|} \cdot \lambda_{laminar} \cdot A_{crosssection} \cdot \sqrt{\frac{2 \cdot p_{max}}{R \cdot T}} \cdot \sqrt{(p_2 - p_1)} \tag{4}$$

$$with\ p_{max} = \begin{cases} p_1\ if\ p_1 \geq p_2 \\ p_2\ if\ p_1 < p_2 \end{cases}$$

4 MODELLING OF MIXED FLOW MEDIUM

For the use of the simulation model in the fuel cell application it is necessary that the gas composition of the media needs to be calculated accordingly. To calculate the specific heat capacity c_p , flow factor c_v, density ρ and dynamic viscosity η the respective mass fractions ω_i are used.

Using mass fractions, the following equation is used to calculate the heat capacity of the mixed media:

$$c_{p_{mix}}(T) = \sum \left(\omega_i \cdot c_{p_i i}(T) \right) \tag{5}$$

$$M_{mix} = \frac{1}{\sum \left(\frac{\omega_i}{M_i} \right)} \tag{6}$$

The molar mass of the mixed media in equation 6 is used for the calculation of the flow factor by:

$$c_{v_{mix}} = c_{p_{mix}} - \left(\frac{R}{\bar{M}_{mix}} \right) \tag{7}$$

For the calculation of the pipe friction coefficient $\lambda_{\mathrm{laminar}}$ the calculation of the density and the dynamic viscosity is necessary.

$$\rho_i(p,T) = \rho_n \cdot \frac{p}{p_n} \cdot \frac{T_n}{T} \tag{8}$$

$$\rho_{mix}(p,T) = \frac{1}{\sum \left(\frac{\omega_i}{\rho_i(p,T)} \right)} \tag{9}$$

$$\Phi_{i,j}(T) = \frac{1}{2 \cdot \sqrt{2}} \cdot \left(1 + \left(\frac{M_i}{M_j} \right) \right)^{-0.5} \cdot \left(1 + \left(\frac{\eta_i(T)}{\eta_{j(T)}} \right)^{0,5} \cdot \left(\frac{M_j}{M_i} \right)^{0,25} \right)^2 \tag{10}$$

$$\eta(T) = \eta_n \cdot \sqrt{\frac{T}{T_n}} \tag{11}$$

$$\eta_{mix}(T) = \sum \left(\frac{x_i \cdot \eta_i(T)}{\sum \left(x_j \cdot \Phi_{i,j}(T) \right)} \right) \tag{12}$$

Equations 8 to 12 lead to the calculation of the Reynolds number under laminar conditions with the assumptions already mentioned in chapter 3:

$$D_H = 4 \cdot \frac{A}{U} \tag{13}$$

$$Re = \frac{D_H \cdot \rho_{mix}(p,T) \cdot v_m}{\eta_{mix}(T)} \tag{14}$$

$$\lambda_{laminar} = \frac{64}{Re} \tag{15}$$

5 MODELLING OF COMPRESSOR

The approach to model the compressor in the fuel cell system cathode path under the given conditions is the “rotating disk” model [1]. For this approach the above-mentioned reservoirs and flows are used for the simulation of the rotating disk approach (Figure 3).

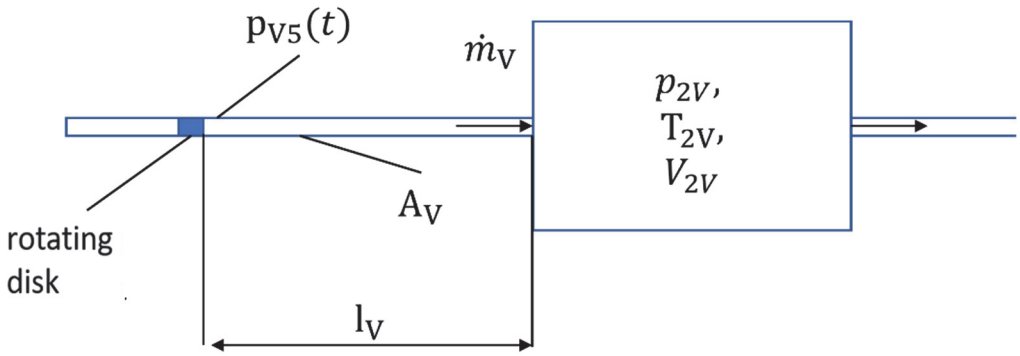

Figure 3: Modelling approach rotating disk, Modell II [1].

In this work the modelling approach of the rotating disk is modified due to the used compressor characteristic diagram. The approach is modified with use of a reservoir which is directly connected to the rotating disk. In [1] both approaches are mentioned as model 1 and model 2 of the compressor model. Model 1 describes the calculation of the compressor mass flow dependent on the total pressure ratio and the compressor speed. Model 2 describes the pressure ratio dependent on the compressor mass flow and compressor speed (equations 16,17).

$$Model\ I\colon\ \dot{m}_{V,bez} = f_I(\Pi_{Vt}, n_{Ver}) \tag{16}$$

$$Model\ II\colon\ \Pi_{Vt} = f_I(\dot{m}_{V,bez}, n_{Ver}) \tag{17}$$

Therefore, the modelling approach of the rotating disk is modified to the mentioned structure.

Figure 4: compressor model I.

For the usage of model 1 the following compressor characteristic estimation is used to generate the compressor characteristic diagram. For developing compressor characteristic diagram module scipy is used to generate a python grid which is able to estimate the compressor characteristic curve for different rotational compressor speeds [3]. With the use of the grid method of scipy the following grid is produced for an exemplary compressor characteristic.

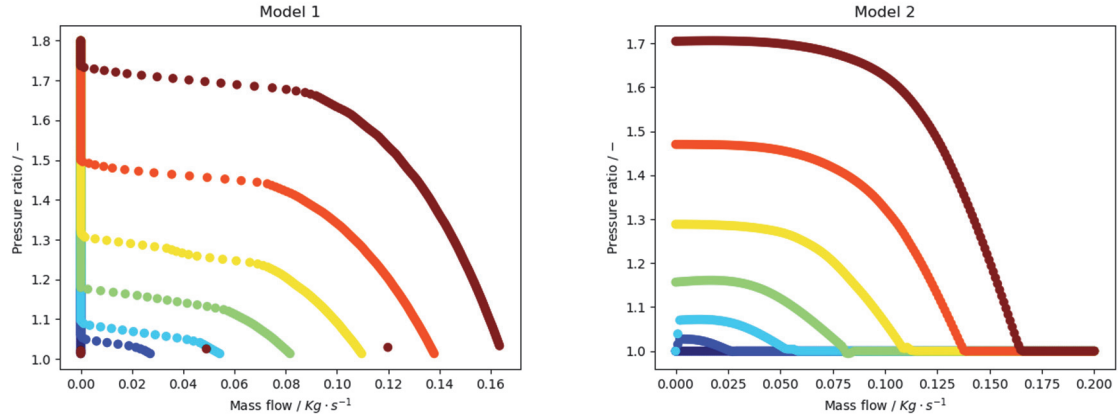

Figure 5: Compressor characteristic diagram.

For the calibration of the current compressor speed and estimated mass flow through the compressor the following approximation for the mass flow of the compressor (model 1) is used.

$$p_{V5} = p_2 + p_0 \cdot \dot{m}_{V,bez}^{p_1} \tag{18}$$

The approximation is used because of various calibration tests from linear regression and exponential regression tests. The approximation is the result of a regression analysis and calibration process. From equation 18 the mass flow is calculated by the use of the equation 3 of the current pressure at the rotating disk.

$$\dot{m}_{V,bez} = \lambda_{laminar} \cdot A_{crosssection} \cdot \sqrt{\frac{2 \cdot p_{V5}}{R \cdot T}} \cdot \sqrt{(p_{V5} - p_{V2})} \tag{19}$$

6 MODELLING OF FUEL CELL

The fuel cell model is divided in different sub models, for calculation of the flow fields, cell voltage and thermal management. Derived from the voltage model described by Gößling in a 2D-1D Model, a reduced model is implemented, that lacks a few key features as no segmentation along the gas paths and the membrane does not serve as a water reservoir [4]. The membrane humidity is solely based on the mean relative humidity of the media in the flow fields. Which functionality is described in section 3 and 4 of this paper.

Waste heat and stack temperatures are calculated on the stack voltage and stack current. Using the provided coolant mass flow, the resulting temperature change for the stack and coolant is calculated by

$$dT_{stack} = \frac{\dot{Q}_{stack} + \dot{Q}_{cool}}{M_{stack} \cdot c_{p_{stack}}} \cdot dt \tag{20}$$

With waste heat $\dot{Q}_{stack}$, provided coolant flux $\dot{Q}_{cool}$, thermal mass and heat capacity of the fuel cell stack M_{stack} and $c_{p\ stack}$. No pressure drop is calculated by thermal management. In addition, the outlet temperatures for the gas flows is set to the stack temperature. This temperature change is not respected by the thermal management yet.

7 MODELLING OF FRONT- AND BACKEND

Based on the simulation model which is based on python module, the frontend and backend architecture of the black box modelling approach is also based on python modules called Dash and Flask. Flask is used to build the architecture for frontend and backend and Dash is used to illustrate the simulation data. Dash is using Flask as architecture to set up frontend and backend. This allows to use call backs of the frontend to get the functionality of the backend.

Due to the usage of the mentioned applications the functionality of starting and stopping, switching between different data to plot as well as downloading all data of the simulation are integrated in the front end shown in Figure 6.

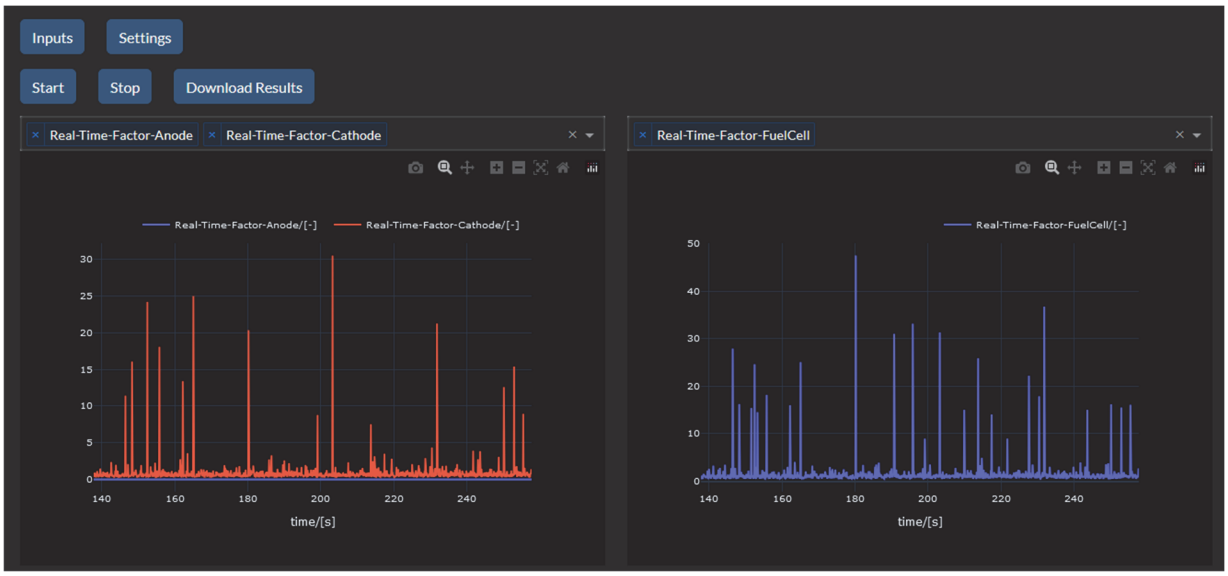

Figure 6: Webinterface of simulation.

8 RESULTS

For the first design of the system simulation only the cathode path of the system has been modelled. In this proof of concept, the simulation time for the cathode path of the fuel cell system was averaging around 0.101 time step of simulation per 0.1 second real time (Figure 7). This indicates that expanding the simulation is possible to achieve a complete simulation of fuel cell systems. Important to notice is that in Figure 7 the limiting factor is the cathode path with the usage of a controller which is transposed from previous works at the ZBT. The usage of this not optimized controller for this application leads to the spikes of the real time factor which leads to a loss of the real time capability of the system. In further work the used controller will be optimized for the web application to deny further limitations of the simulation.

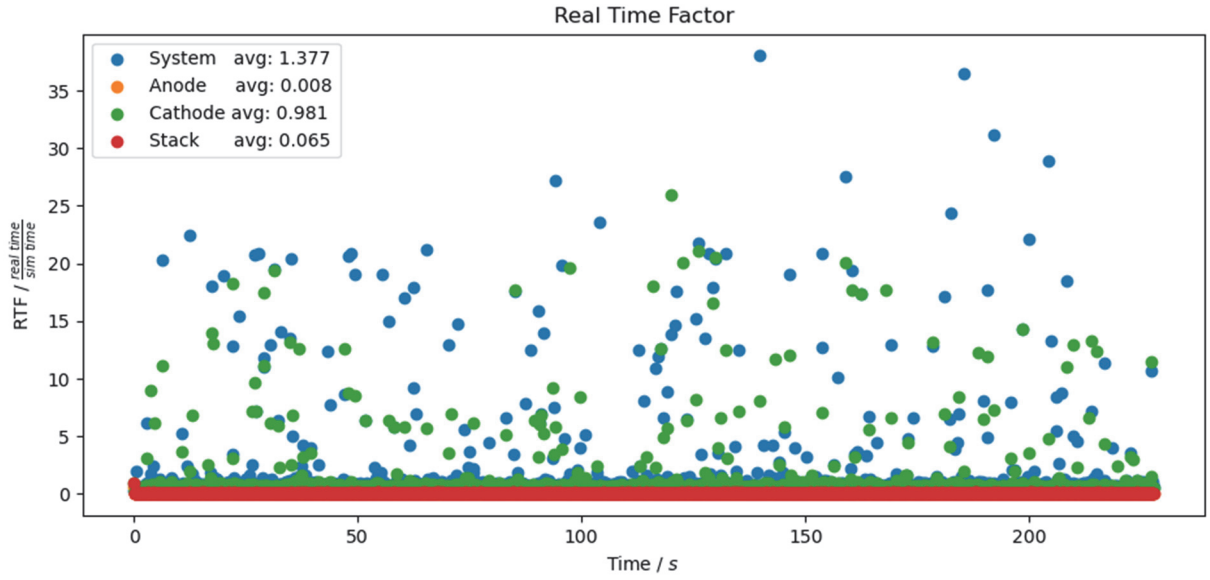

Figure 7: Real-time-factor of cathode, anode and fuel cell stack.

For proving the simulation approach Figure 8 shows a generic load profile of the cathode fuel cell system providing plausibility on a working cathode simulation by ramping up and down the system. In the simulation the approach for simulating the compressor model approach 1 is used to provide the following time dependent simulation data. As results show the system was able to change the load depending on the user's system power setpoint.

Due to the current limitations of the fuel cell simulation the system lowest power point is around 10% of the nominal Power. In this case the fuel cell is calibrated at 150kW nominal power. This behaviour is shown in the first 25 seconds of Figure 8. Significant as well are the limitation of the actual stack power according to the limiting ramp rate of the cathode compressor, which results in a time delayed reaching of the set point of the stack.

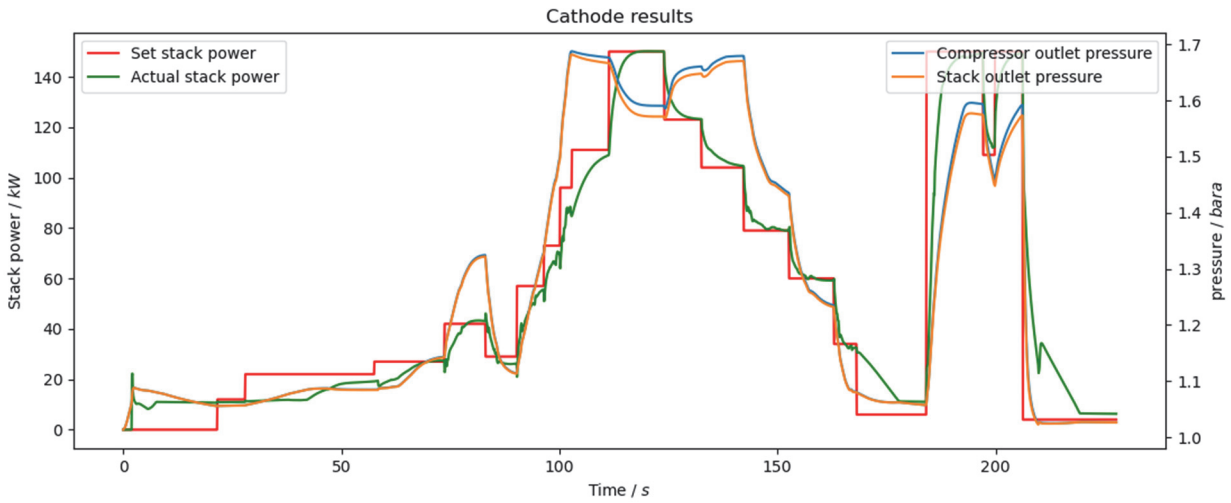

Figure 8: Simulation of Cathode of Fuel Cell.

9 CONCLUSION

The new simulation approach by modelling system components as black boxes shows potential to overcome the issues of high cost due to the open-source approach of the base framework. Achieving runtime of around real time and the behaviour of the compressor and the cathode side of the fuel cell show the potential of this approach of reducing the numerical demands.

Nevertheless, it is more work required to test the simulation environment as well as optimizing more components of the simulation like the mentioned controller. To provide more results and validation of the simulated system further work needs to be done by expanding the systems on a full scale fuel cell system providing data, which are validated by cross validation of the fuel cell system from Gößling [4]. Another point of interest which couldn't be covered, is the simultaneously use of the simulation by different users on the hosted website, due to runtime concerns. Therefore, continues research is needed after publishing the website, to get results of the runtime of the simulation under various operation conditions on the web-based hosting.

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